

**Close out and Final report for
NASA Glenn Cooperative Agreement NCC3-594**

**Title: Computational Materials Program for Alloy Design
PI: Dr. Guillermo Bozzolo**

Introduction

The research program sponsored by this grant, ‘Computational Materials Program for Alloy Design’, covers a period of time of enormous change in the emerging field of computational materials science. With a steady pace, the program not only pioneered some of these changes, but also adapted to the new challenges by reformulating goals and objectives in agreement with new trends and needs. The computational materials program started with the development of the BFS method for alloys, a quantum approximate method for atomistic analysis of alloys specifically tailored to effectively deal with the current challenges in the area of atomistic modeling and to support modern experimental programs. During the grant period, the program benefited from steady growth which, as detailed below, far exceeds its original set of goals and objectives. Not surprisingly, by the end of this grant, the methodology and the computational materials program became an established force in the materials community, with substantial impact in several areas.

Under sponsorship of the HITEMP program at NASA GRC, the BFS-based activity evolved into a multi-disciplinary task linking the efforts of different groups within NASA. In this process, it became a major driving force in the emerging field of computational materials science. These accomplishments were supported with a large number of peer-reviewed journal publications, book chapters, conference proceedings, invited and contributed presentations in domestic and international conferences, software development, and a substantial network of collaborations that today make the BFS-based activity one of the leading methodologies in the market.

Early in this grant period, the materials modeling activity was rewarded with the Distinguished Publication of the Year (1999), bringing substantial visibility and interest from the community. Matched by a continued string of seminal publications in prestigious journals, the activity was quickly established on its way to provide substantial benefits realized later during the grant period. This early achievement was further enhanced by the good reception that the methodology had with leading aerospace companies (Pratt & Whitney, GE, Allison) and their programmatic support, as well as the benefits brought on by a healthy network of associates and collaborators.

Major achievements during the duration of the grant include the completion of a Level 1 Milestone for the HITEMP program at NASA Glenn, consisting of the planning, development and organization of an international conference held at the Ohio Aerospace Institute in August of 2002, finalizing a period of rapid insertion of the methodology in the research community worldwide. The conference, attended by citizens of 17 countries representing various fields of the research community, resulted in a special issue of the leading journal in the area of applied surface science. Another element of the Level 1 Milestone was the presentation of the first version of the Alloy Design Workbench software package, currently known as ‘adwTools’. This

software package constitutes the first PC-based piece of software for atomistic simulations for both solid alloys and surfaces in the market. This task was the result of a joint effort by members of the NASA GRC/OAI Computational Materials Group (CMG), established during this grant period as the means to nucleate the diverse efforts which, on the OAI end, were lead by the P.I.

Contemporary with the completion of the Level 1 Milestone, the P.I. founded the International Computational Materials Science Consortium, which through the years have provided the Computational Materials Group with the ideal means to facilitate collaborations and visits by leading scientists and also helping promote the work done at NASA GRC in the area of computational materials design. As a result, the group grew to its current network of domestic and international collaborations which nurtured further growth in the modeling activity, to levels of productivity unforeseen at the beginning of this effort.

During the last period of this grant, the BFS-based activity grew in unexpected ways, opening new lines of research originally considered to be outside the scope of the proposed work. As a result, the P.I. is now compiling such results and achievements in a book for Kluwer Academic Publishers, which provides a complete description of the state-of-the-art in computational materials science, with a prominent presence of the BFS-based activity as realized during this grant.

Dissemination of results and insertion in the materials community worldwide was a primary focus during this period. As a result, the P.I. was responsible for presenting 37 contributed talks, 19 invited talks, and publishing 71 articles in peer-reviewed journals, as detailed later in this Report.

Milestones

1. Distinguished Publication of the Year, NASA Glenn Research Center, 1999.

The paper "Surface Segregation in Multicomponent Metallic Systems: Surface Alloys and Alloy Surfaces", authored by all the members of the Computational Materials Group (G. Bozzolo, J. Ferrante, R. D. Noebe, B. Good, F. S. Honey and P. Abel), published in Computational Materials Science 15 (1999) 169, received this prestigious award, together with a Group Achievement Award for the year, bringing a heightened level of awareness and recognition of the activity within NASA.

2. Creation of the International Computational Materials Science Consortium (ICMSC)

Lead by the P. I., the original objective of the ICMSC of creating an international network of scientists devoted to the emerging field of computational materials science was fulfilled with the addition of numerous domestic and international partners, and with the development of numerous collaborations, each dealing with the equally diverse topics of interest in the field. The central theme continued to be the consolidation of theory and experiment, and the insertion of computational modeling as the necessary link between them. As a result, a substantial number of collaborative efforts were initiated, maximizing the available knowledge and resources. While

diverse in nature, all current projects are firmly defined within the unifying goal of introducing computational modeling as a major tool in materials design and analysis. Current members include the founding group -CMG-, as well as individuals from the Universidad Autonoma de Madrid (Spain), Katholieke Universiteit Leuven (Belgium), University of Ioannina (Greece), Universidad Nacional Autonoma de Mexico (Mexico), Comisión Nacional de Energía Atómica (Argentina) and Montana State University (USA).

3. A Level 1 Milestone for the HOTPC project was successfully completed with the unveiling of the Alloy Design Workbench – Surface Modeling Package (ADW-SMP) software at the ‘Applied Surface Modeling: Experiment, Theory, and Simulations’ (ASM-ETS) conference held at OAI, August 20-23, 2002. As Chairman of the International Computational Materials Science Consortium (ICMSC), sponsored and funded by HOTPC, the P.I. was responsible for the organization, planning and development of the conference. In parallel with these developments, a major research effort in computational atomistic modeling of alloys and surfaces was carried out, in collaboration with numerous partners, resulting in a record number of journal publications and international conference presentations. This effort, in addition to its intrinsic scientific value, established the necessary foundation to the ADW-SMP computational tool by providing the theoretical background and applications needed to validate the underlying theory (the BFS method for alloys, the universal parameterization with first-principles methods, etc.), and the numerous aspects related to the functionality of the software.

As the main outreach activity of the ICMSC for 2001-2002, the ASM-ETS conference was held at OAI, August 20-23, 2002. Representatives of 17 countries attended the conference, each providing a different angle to the numerous aspects that characterize the integration of theory, experiment and computational modeling in the field of alloy surfaces and surface alloys. Distinguished invited speakers defined a solid framework for the conference, with detailed overviews of the achievements and difficulties facing this emerging field. The conference included 11 invited talks, 21 contributed talks and over 20 posters. The social program included a banquet at the Great Lakes Science Center. The conference was held at OAI, which provided the necessary facilities and personnel for its organization and successful development. The creation of the ICMSC, the software release, and the ASM-ETS conference organization were the result of the combined effort of the Computational Materials Group (CMG), a multidisciplinary team with members of OAI (G. Bozzolo, J. Khalil, J. Morse) and NASA (R. D. Noebe, P. Abel, B. Good).

4. Alloy Design Workbench – Surface Modeling Package (ADW-SMP)

As part of the Level 1 Milestone for the HOTPC project, the ADW-SMP was completed and introduced at the ASM-ETS conference. ADW-SMP fulfills the need of performing, in a seamless fashion, detailed atom-by-atom calculations with large scale atomistic simulations, using different statistical methods for performing ‘computer experiments’, all using the BFS method for alloys as the engine for the calculation of the energetics. The graphical user interface (GUI) was especially designed for use by experimentalists with no previous experience in computational modeling methods, thus bringing a highly desirable degree of versatility for its application and intended use. The software, written in Java and FORTRAN 90, is equally

supported by unix workstations and desktop PC's, providing results in real time. Testing by ICMSC members with experimental background was a cornerstone in the development of the package, resulting in maximum ease of use and insertion as a laboratory tool.

5. adwTools nanostructure modeling package

One major accomplishment during this grant period was the planning, design, development and implementation of the 'Alloy Design Workbench Tools' (adwTools) software package. The package provides a simple PC-based platform for performing detailed atomistic analysis of multicomponent alloys and their surfaces, at the nanometer scale, using the BFS method for alloys. The graphical user interface provides a simple, straightforward and efficient tool for adding computational modeling to experimental alloy design. During this period, the activity focused on beta-testing this package by a number of international partners, thus enhancing their scope, capabilities, and usability. The release of *adwTools* v2.8 to the international users group further enhanced collaborative efforts between our computational materials group and other institutions worldwide. The network of beta-testers of *adwTools* provided continued and invaluable input for further enhancements and additions to the software package. Routine updates were made and distributed to the users, which in turn provided us with constant revisions and suggestions for optimizing the package's capabilities. Several limitations of the software were eliminated and its scope of application greatly expanded. A first version of the *adwTools* Users Manual was developed and distributed to selected users for further input and suggestions. The code fulfills the need of performing, in a seamless fashion, detailed atom-by-atom calculations with large scale atomistic simulations, using different statistical methods for performing "computer experiments," all using the BFS method for alloys as the engine for the calculation of the energetics. The graphical user interface (GUI) was especially designed for use by experimentalists with no previous experience in computational modeling methods, thus bringing a highly desirable degree of versatility for its application and intended use. The software, written in Java and FORTRAN 90, is equally supported by unix workstations and desktop PC's, providing results in real time. Testing by experts with experimental background was a cornerstone in the development of the package, resulting in maximum ease of use and insertion as a laboratory tool.

6. adwParams software for BFS parameterization

A second software package, 'Alloy Design Workbench: Parameterization' for internal use was developed by the OAI team to provide accurate and reliable parameterization for adwTools usage. This program is supported with one of the largest elemental databases actually in existence, determined via first-principles calculations. Together with adwTools, this package is the essential tool for accurately representing a large number of elements needed for the several topics of research amenable to BFS calculations.

7. adwReport, a central repository for adwTools and adwParams results

A third piece of software has been developed to support and document adwParams and adwTools input and output. This report, accessible by adwTools users, provides a unified platform for exchange of information and data gathering, besides its primary goal of serving as a repository of modeling data (input parameters, analysis, testing and validation). This activity became the centerpiece of the computational effort during the last stages of the grant period, leading to the largest database of interaction parameters which enable the application of the methodology to countless multicomponent systems. This is, by any measure, the largest database available among current methods, further establishing the computational materials group activity as a leader in the field. Future proposal periods will continue to focus the interactive adwReport database, by making it accessible by all users of any module of the adwTools package.

8. Computational Materials Group (CMG)

During the grant period, the CMG expanded its original operational base with the addition of two members, Joseph Khalil and Jeff Morse, each bringing necessary skills to the software and GUI development task. Both members were under the supervision of the P.I. and joined OAI as Research Assistants. Joseph Khalil was instrumental in efficiently tackling the increased workload of the CMG, providing much needed assistance in the development of software, computer networking, scientific research, and organization of the ASM-ETS conference. Jeff Morse was responsible for the development of an advanced GUI for adwTools. A summer intern, Adam Busony, contributed to the adwTools effort with the production of a stand-alone GUI for the visualization of adwTools results, helping also in the development of the ASM-ETS conference website.

9. The BFS method for alloys

The main tool to be used in this work is the Bozzolo-Ferrante-Smith (BFS) method for alloys and the Equivalent Crystal Theory (ECT) for pure materials. These methods, based on sound physical theories, provide the mechanism for performing large scale atomistic computer simulations of metals and their alloys. In the field of computational materials science at the atomic length scale, the BFS method stands alone as the only one capable of efficiently dealing with multicomponent systems in any crystallographic structure. Recent progress and planned work for the upcoming period substantiate its potential for being the method of choice for realistic large-scale simulations delivering specific properties useful for alloy design and analysis. The engine of all the work described above is the BFS method for alloys, developed by the P.I. and coauthors in 1992. While the foundation of the method was firmly established by the beginning of this grant period, several enhancements and extensions were implemented during the years, making it today the only available quantum approximate method capable of dealing with multicomponent alloys without limitation in the number and type of elements. During the years, the effort of further developing the method was aided by essential collaborations carried out under the sponsorship of the International Computational Materials Science Consortium.

10. Collaborations

An essential ingredient furthering the development of the activity was the sustained support of a large network of collaborations domestically and internationally. With the goal of establishing a multinational group of users of the adwTools package, collaborative efforts maximizing the available knowledge and resources were nurtured and pursued during this period. While diverse in nature, all current projects are firmly defined within the unifying goal of introducing computational modeling as a major tool in materials design and analysis. The different projects include interactions with individuals from the Universidad Autonoma de Madrid (Spain), Katholieke Universiteit Leuven (Belgium), Loyola College (USA), Comision Nacional de Energia Atomica (Argentina), Montana State University (USA), and Clark Atlanta University (USA). In addition, the PI directed theses and supervised summer interns at NASA GRC throughout the grant period.

11. Technical Accomplishments

With the development of the BFS method for alloys, and the production of its associated software, initial goals for the application of modeling techniques was greatly expanded from its original goal of understanding simple high temperature intermetallic systems, to cover a large range of topics. Some highlights, where the BFS-based activity has far met its promise as an efficient tool for supplementing experimental work include:

11. a High temperature intermetallics: Starting with detailed understanding of the defect structure of NiAl, the methodology far exceeded its original goal by providing new insight on the role of multiple alloying additions, the microscopic description of the resulting structures as well as their surface properties.

11. b Surface alloys and Alloy surfaces: A great deal of effort was devoted to the first detailed analysis of alloy surfaces and surface alloys, which exceeds current experimental knowledge. This area of research became a major component of the modeling activity, leading to some of the most striking results, as detailed in the list of publications below.

11.c High Temperature Shape Memory Alloys: With all the components of the modeling program in place, substantial effort and groundbreaking results were brought forward in the development of shape memory alloys for high temperature applications. This novel activity was performed in conjunction with experimental work by the Materials Division at GRC, marking the first time in which computational modeling realized its promise as a predictive tool for alloy design with substantial savings in time, effort, and experimental work, while at the same time providing the guidance necessary for understanding, at every step, the relevant features of these materials.

11.d Superalloys: Another groundbreaking milestone was achieved by the modeling effort by supplementing experimental work dealing with unexpected progress in the development of new superalloys, where incremental changes had far limited further growth in the area via traditional experimental work.

11.e Nuclear materials: Perhaps the most unexpected outgrowth of the modeling activity consists of the rather recent insertion of the BFS-based methodology for further understanding and development of nuclear materials for reduced-enrichment research and test reactors. In this case, the modeling activity not only reproduced results obtained experimentally but also provided the necessary understanding for the observed behavior. Moreover, the modeling tools constitute now the driving force for the design of new experiments and further development of low-enriched nuclear fuels.

12. Publications and presentations

12.a Contributed talks

1. Development of a Computational Modelling Method for Alloy Design

G. Bozzolo and R. D. Noebe

HITEMP Conference

Cleveland, OH, April 1997.

2. Computational Modelling Method for Superalloys

Propulsion Materials and Structures Symposium

Cleveland, OH, April 1997.

3. Atomistic Simulations of Alloying Additions to NiAl

G. Bozzolo, R. D. Noebe, J. Ferrante and A. Garg

4th International Conference on High Temperature Intermetallics

San Diego, CA, April 1997.

4. Progress in the Modelling of NiAl-based Alloys using the BFS Method

G. Bozzolo, R. D. Noebe, J. Ferrante and A. Garg

International Symposium on Structural Intermetallics

Champion, PA, September 1997.

5. Computer Modeling of Intermetallics

G. Bozzolo and R. D. Noebe

9th International Conference on Modern Materials and Technologies, CIMTEC 98

Florence, Italy, June 1998

6. Evolution of a Computational-Based Alloy Design Tool for the Development and Understanding of High Temperature Structural Alloys.

G. Bozzolo and R. D. Noebe

HITEMP Conference

Cleveland, OH May 1999

7. Surface Segregation in Ternary Alloys

G. Bozzolo, B. Good and P. Abel

**18th European Conference on Surface Science
Vienna, Austria, September 1999**

8. Surface Alloys of (Cu.Au)/Ni(110)

G. Bozzolo, J. Garces and H. Mosca

**18th European Conference on Surface Science
Vienna, Austria, September 1999**

9. Surface Segregation in Multicomponent Systems: Modeling of Surface Alloys and Alloy Surfaces

G. Bozzolo, J. Ferrante, R. D. Noebe, B. Good, F. Honey and P. Abel

**Surface Analysis 2000
Penn State University, PA, June 2000**

10. Formation of Pd-Cu Surface Alloys

H. Mosca, J. Garces, G. Bozzolo and P. Abel

**Sociedad Argentina de Materiales 2000
Comahue, Argentina, August 2000**

11. Surface Alloys of Pd and Cu via Atomistic Modeling

G. Bozzolo, J. Garces, H. Mosca and P. Abel

**19th European Conference on Surface Science
Madrid, Spain, September 2000**

12. Atomistic Modeling of Ternary and Quaternary Ordered Intermetallic Alloys

G. Bozzolo, J. Khalil, M. Bartow and Ronald. D. Noebe

**Materials Research Society Fall Meeting
Boston, MA, November 2000**

13. Bulk and Surface Structure of Alloys Via BFS Atomistic Monte Carlo Simulation

B. Good and G. Bozzolo

**2001 Annual Meeting of the Division of Computational Physics
Massachusetts Institute of Technology, Cambridge, MA, June 2001**

14. Modeling of 3C-SiC(100) using the BFS Method for Alloys

G. Bozzolo, J. Garces and P. Abel

**20th European Conference on Surface Science
Krakow, Poland, September 2001**

15. Surface Composition of Alloys via BFS Atomistic Monte Carlo Simulations

B. Good and G. Bozzolo

**20th European Conference on Surface Science
Krakow, Poland, September 2001**

16. Atomistic Modeling of Co Growth on Cu(111)

J. Khalil, G. Bozzolo, D. Farias, A. Vazquez de Parga, J. J. de Miguel and R. Miranda
Materials Research Society Fall Meeting
Boston, MA, November 2001

17. Atomistic Modeling of Co growth on Cu(111)

D. Farias, A. L. Vazquez de Parga, J.J. de Miguel, R. Miranda, J. Khalil and G. Bozzolo
TMR Meeting
Leuven, Belgium, October 2001

18. Modeling of Co/Cu island formation on a Cu(111) surface

J. Khalil, G. Bozzolo, D. Farias, A. Vazquez de Parga, J. J. de Miguel and R. Miranda
Surf. Sci. (2002) (submitted)
21st European Conference on Surface Science
Malmo, Sweden, June 2002

19. Atomistic Modeling of Au deposition on a Cu substrate

G. Bozzolo, J. E. Garces and G. Demarco
21st European Conference on Surface Science
Malmo, Sweden, June 2002

20. Theoretical Description of the Deposition of Al on the UMo Solid Solution

J. Garces, G. Bozzolo and A. Marino
Applied Surface Modeling: Experiment, Theory, and Simulations
Cleveland, OH, August 2002.

21. Atomistic Description of the Coverage Dependent Structural Phase Transition in the Sn/Cu(100) System

G. Bozzolo and J. E. Garces
Applied Surface Modeling: Experiment, Theory, and Simulations
Cleveland, OH, August 2002.

22. Surface Composition of Ni-Pd Alloys

R. D. Noebe, J. Khalil and G. Bozzolo
Applied Surface Modeling: Experiment, Theory, and Simulations
Cleveland, OH, August 2002.

23. Atom-by-atom description of the process of mixed Co-Cu island formation on a Cu substrate

G. Bozzolo and D. Farias
Applied Surface Modeling: Experiment, Theory, and Simulations
Cleveland, OH, August 2002.

24. Tools for atomistic modeling of surfaces

G. Bozzolo

Applied Surface Modeling: Experiment, Theory, and Simulations

Cleveland, OH, August 2002.

25. Heats of segregation of bcc metals using ab initio and quantum approximate methods

B. Good, A. Chaka, G. Bozzolo

American Physical Society March Meeting

Austin, TX, March 2003

26. Experiment and Modeling of Co and Fe Superlattices grown on Cu(111)

D. Farías, M. A. Niño, J. J. de Miguel, R. Miranda and G. Bozzolo

11th International Symposium on Nanostructures

St. Petersburg, Russia, June 2003

27. Experiment and Modeling of Co and Fe Superlattices grown on Cu(111)

D. Farías, M. A. Niño, J. J. de Miguel, R. Miranda and G. Bozzolo

29th IUVESTA Workshop on Gas-phase Cluster Assembling of Nanostructured Materials

Erice, Italy, July 2003

28. Experiment and Modeling of Co and Fe Superlattices grown on Cu(111)

D. Farías, M. A. Niño, J. J. de Miguel, R. Miranda and G. Bozzolo

18th International Colloquium on Magnetic Films and Surfaces

Madrid, Spain, July 2003

29. Experiment and Modeling of Co and Fe Superlattices grown on Cu(111)

D. Farías, M. A. Niño, J. J. de Miguel, R. Miranda and G. Bozzolo

22nd European Conference on Surface Science

Prague, Czech Republic, September 2003

30. Tools for Atomistic Modeling of Alloys

G. Bozzolo

Center for the Theoretical Study of Physical Systems

Clark Atlanta University

Atlanta, GA, October 2003

31. Surface segregation in multicomponent metallic alloys

P. Gargano, H. Mosca and G. Bozzolo

Sociedad Argentina de Metales (SAM)

Bariloche, Argentina, November 2003

32. Atomistic Modeling of Interdiffusion Barriers in the Interphase Al/UMo-Based Fuel
J. E. Garcés, G. Demarco and G. Bozzolo
International Conference on Research Reactor (Utilization, Safety, Decommissioning, Fuel, and Waste Management)
Santiago, Chile, November 2003
33. Theoretical Study of the Structural Order in the Fe/Cu System
G. Demarco, J. E. Garcés, H. E. Troiani and G. Bozzolo
Jornadas SAM - Simposio Materia 2003 - Congreso CONAMET
Bariloche, Argentina, November 2003
34. Atomistic Modeling of the interdiffusion of Al in UMo-based fuels
J. E. Garcés, A. Marino, G. Bozzolo
Jornadas SAM - Simposio Materia 2003 - Congreso CONAMET
Bariloche, Argentina, November 2003
35. Substrate Orientation Dependence of Interface Alloy Formation for Ni Films in Al Single Crystals. Comparisons of Monte Carlo Simulations with Experiment
R. J. Smith, N. Winward, C. V. Ramana, V. Shutthanandan, N. R. Shivaparan, Y.-W. Kim and G. Bozzolo
American Vacuum Society Fall Meeting 2003
Baltimore, MD, November 2003
36. Atomistic Modeling of Ta Site Preference in RuAl
P. Gargano, H. Mosca, G. Bozzolo
Sociedad Argentina de Materiales y Metales
Santiago de Chile, Chile, November 2004
37. Modeling of the surface alloys Pd/Cu(111), Pt/Cu(111) and Cu/Pt(111)
G. Bozzolo, H. Mosca and A. Canzian
Sociedad Argentina de Materiales y Metales
Santiago de Chile, Chile, November 2004

12.b Invited talks

1. Atomistic Simulations as Tools for Alloy Design
Case Western Reserve University, April 1997.
2. Atomistic Simulations as Tools for Alloy Design
Pratt & Whitney, West Palm Beach, FL, June 1997.
3. Application of the BFS Method to Metallic Surfaces: Surface Alloys and Alloy Surfaces
G. Bozzolo
School on Surfaces, Comision Nacional de Energia Atomica, Buenos Aires, Argentina, July 1997.

4. Modeling of Substitutional Site Preference in Ordered Intermetallic Alloys
G. Bozzolo, R. D. Noebe and F. Honey
Symposium Interstitial and Substitutional Effects in Intermetallics
Fall Meeting of The Minerals, Metals and Materials Society, Rosemont, IL, October 1998.
5. The Role of Computational Modeling Processes in the Development and Understanding of
NiAl-based Ordered Intermetallic Alloys
Materials Research Society Fall Meeting,
Boston, MA, November 1998.
6. Monte Carlo Prediction of Alloy Structure
B. Good and G. Bozzolo
Materials Research Society Fall Meeting,
Boston, MA November 1998.
7. Computational Materials Science: The BFS Method
Centro Atomico Bariloche, Comision Nacional de Energia Atomica, Bariloche, Argentina,
April 1999.
8. Atomistic Simulations of Multicomponent Intermetallics and Superalloys
Naval Research Laboratory, Washington, DC, May 2000
9. BFS Atomistic Modeling of Surface Alloys and Alloy Surfaces
Universidad Autonoma de Madrid, Madrid, Spain, February 2001
10. Atomistic Modelling of Surfaces via Quantum Approximate Methods
G. Bozzolo
Applied Surface Modeling: Experiment, Theory, and Simulations
Cleveland, OH, August 2002
11. Atomistic Modeling of Nanostructures via Quantum Approximate Methods
Trends in Nanotechnology 2002
Santiago de Compostela, Spain, September 2002
12. Developing Tools for Atomistic Modeling in Materials Science
Montana State University
Bozeman, MT April 2003
13. Atomistic Modeling of Alloys
Montana State University
Bozeman, MT April 2003
14. adwTools: Atomistic Modeling in Materials Science
Clark Atlanta University
Atlanta, GA October 2003

15. Developing Tools for Atomistic Modeling in Materials Science
Universidad Autónoma de Madrid
Madrid, Spain, November 2003

16. Developing Tools for Atomistic Modeling in Materials Science
Katholieke Universiteit Leuven
Leuven, Belgium, December 2003

17. Quantum Approximate Methods for Atomistic Modeling of Alloys
Comisión Nacional de Energía Atómica
Buenos Aires, Argentina, June 2004

18. Atomistic Modeling of Nuclear Materials
Argonne National Laboratory
Argonne, IL, June 2004

19. Atomistic Modeling of Interfaces
Gordon Research Conference
Watersville, ME, August 2004

12.c Refereed publications in print

1. Alloy Surface Structure: Computer Simulations using the BFS Method
G. Bozzolo and J. Ferrante
Surf. Rev. Lett. 4 (1997) 825

2. Energetics of Ternary and Quaternary Alloy Surfaces
G. Bozzolo, J. Ferrante and R. D. Noebe
Surf. Sci. 377-379 (1997) 1028

3. Modelling of Thin Films via a Semiempirical Method
G. Bozzolo and J. Ferrante
Thin Solid Films 317 (1998) 1

4. Atomistic Simulations of Ti Additions to NiAl
G. Bozzolo, R. D. Noebe, A. Garg, J. Ferrante and C. Amador
Mat. Res. Soc. Symp. Proc. 460 (1997) 443

5. Zero Temperature Analysis of the Defect Structure of B2 FeAl Alloys
G. Bozzolo, J. Ferrante, R. D. Noebe and C. Amador
Scripta Metall. 36 (1997) 813

6. Progress in the Modelling of NiAl-based Alloys using the BFS Method
G. Bozzolo, R. D. Noebe, J. Ferrante and A. Garg
Structural Intermetallics 1997, M. V. Nathal, ed. , The Minerals, Metals and Materials Society, Warrendale, PA 1997.
NASA Technical Memorandum 113117
7. Atomistic Simulations and Experimental Analysis of the Effect of Ti additions on the Structure of NiAl
G. Bozzolo, R. D. Noebe, J. Ferrante, A. Garg and C. Amador
NASA Technical Memorandum (1997) 113121.
8. Modelling of Alloy Surfaces
G. Bozzolo, J. Ferrante, F. Honey and R. D. Noebe
Surf. Sci. (1997) (submitted)
NASA Technical Memorandum
9. Atomistic Simulations of Alloying Additions to NiAl
G. Bozzolo, R. D. Noebe, J. Ferrante and A. Garg
Proc. of the 4th International Conference on High Temperature Intermetallics
Materials Science and Engineering A 239-240 (1997) 769.
NASA Technical Memorandum 113119, September 1997.
10. Surface Segregation in Ternary Alloys: A BFS Study of Ni-Al-Cu (100) Surface Composition
F. Honey, G. Bozzolo and B. Good
Applied Surface Science 137 (1999) 157.
11. A BFS Survey of Surface and Interfacial Properties of Multicomponent Metallic Systems
G. Bozzolo and J. Ferrante
Mat. Res. Soc. Symp. Proc. 492 (1998)
'Microscopic Simulation of Interfacial Phenomena in Solids and Liquids'
S. R. Philpot, P. D. Bristowe, D. G. Stroud and J. R. Smith, eds.
12. An Introduction to the BFS Method and its use to Model Binary NiAl Alloys
G. Bozzolo, R. D. Noebe, J. Ferrante, A. Garg and C. Amador
J. Computer-Aided Mater. Design 6 (1999) 1
NASA TM 208820-1998
13. Atomistic Simulations and Experimental Analysis of Ti Additions to NiAl Alloys
G. Bozzolo, R. D. Noebe, J. Ferrante, F. Honey and A. Garg
J. Computer-Aided Mater. Design 6 (1999) 33

14. Computer Modeling of Intermetallics

G. Bozzolo and R. D. Noebe

in Advances in Science and Technology, Vol. 18

Computational Modeling and Simulation of Materials

CIMTEC'98 Proceedings, pp. 463-470.

P. Vincenzini and A. Degli Esposti, eds.

Techna Srl, Faenza, Italy 1999.

15. Modeling of Substitutional Site Preference in Ordered Intermetallic Alloys.

G. Bozzolo, R. D. Noebe and F. Honey

Interstitial and Substitutional Effects in Intermetallics

The Minerals, Metals and Materials Society, Warrendale, PA, 1998.

NASA Technical Memorandum 208665.

16. Monte Carlo Prediction of Alloy Structure

B. Good and G. Bozzolo

Mat. Res. Soc. Symp. Proc. 551 (1999).

17. The Role of Computational Modeling Processes in the Development and Understanding of NiAl-based Ordered Intermetallic Alloys

G. Bozzolo, R. D. Noebe, F. S. Honey and B. Good

Mat. Res. Soc. Symp. Proc. 552 (1999) 693.

18. Surface Segregation in Multicomponent Metallic Systems: Surface Alloys and Alloy Surfaces

G. Bozzolo, J. Ferrante, R. D. Noebe, B. Good, F. S. Honey and P. Abel

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